# Characterizing Natural Organic Material from the Occoquan Watershed (Northern Virginia, US) using Fluorescence Spectroscopy and PARAFAC

*Surface water samples from the Occoquan Watershed (Virginia, US) were collected during summer baseflow conditions and characterized by excitation-emission matrix (EEM) fluorescence spectroscopy and parallel factor analysis (PARAFAC). Based on 55 samples, PARAFAC identified three individual fluorophore components, which were attributed to humic-like, fulvic-like, and protein-like materials. The NIST-led research team demonstrated that PARAFAC can be used to provide estimates (± 30%) of select analyte concentrations in surface water.*

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Three individual fluorophore components were categorized in surface water samples from the Occoquan Watershed using excitation-emission matrix (EEM) fluorescence spectroscopy and parallel factor analysis (PARAFAC). The concentrations of these three seemingly universal fluorophore components in aqueous systems were consistent with expected analyte concentrations that were independently measured by traditional wet chemistry techniques. The relative distribution of the three fluorophore fractions varied among the different land use catchments, especially in locations of known anthropogenic activity (Figure 1). Distinctive relationships between the fulvic-like and protein-like materials were observed for catchments known to be influenced by anthropogenic activity and those believed to reflect more natural environments, suggesting that this technique could be used to monitor human impact on aquatic systems.

The results of this work address three aspects of fluorophore characteristics and PARAFAC analysis of organic matter obtained from surface water samples within the Occoquan Watershed: 1) the presence of similar, universal fluorophore moieties in aqueous systems whose categorization is consistent with traditional wet chemistry analysis; 2) the variability in water quality caused by different land use catchments, especially in areas of concentrated human activity and/or urbanization; and 3) the ability of PARAFAC to capture and predict concentrations of selected aqueous analytes.

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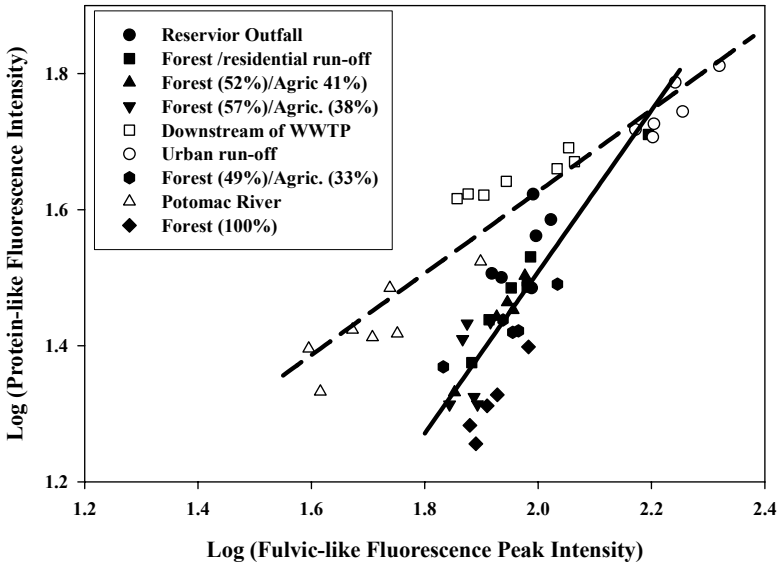
These experiments support the use of EEM and PARAFAC analyses by watershed managers and other personnel interested in understanding organic matter behavior especially that derived from anthropogenic activity, in aquatic systems.

***Future Plans***: A proposal has been submitted with VA Tech to the Cooperative Institute for Coastal and Estuarine Environmental Technology (CICEET) to develop similar detection and analysis techniques to control a small, long-endurance autonomous surface vehicle system (ASV) that will be developed by VA Tech researchers. This would allow continuous mapping and tracking of organic matter distributions in three dimensions over periods of up to one week.




***Logarithmic correlation between scores of protein-like and fulvic acid-like fluorophores. The open symbols include locations known to be influenced by anthropogenic activity (y = 0.42 + 0.60(x), $r^2$ = 0.92) while the filled symbols are indicative of more natural environments (y = -0.87 + 1.19(x), $r^2$ = 0.65).***